Final Report for Grant Number: FA9550-04-1-0235 New Meta Algorithms for Engineering Design Using Surrogate Functions

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14. ABSTRACT

We have recently made an important breakthrough in both the theory and the practice of derivative-free methods. Our new research eliminates the main limitation of the Generalized Pattern Search (GPS) class of algorithms, which formed the algorithmic infrastructure for our past work. Our new work addressed the issue that the GPS algorithm class relies heavily on a fixed finite set of directions, and that the convergence results are heavily tied to these directions. We found a way to lift these restrictions, and now we allow the algorithm to explore in a set of directions which is dense in the entire space. We call this the Mesh Adaptive Direct Search (MADS) class of algorithm, and it generalizes GPS. we observed significant improvements on some interesting problems.

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Status of Effort:

This contract represents a one year increment to the three year contract F49620-01-1-0013.

In May 2004, Exxon-Mobil sponsored the third international workshop on surrogate optimization. This workshop was held at Rice, and it followed the first workshop held at the Danish Technical University and the second held in Coimbra, Portugal. The Rice workshop had participation from several industrial groups, most notably Boeing and ExxonMobil, as well as SANDIA and Lawrence Berkeley Labs. Our former joint PhD student and present collaborator, Lt Col Mark Abramson of AFIT, attended as well.

The papers from the Danish workshop appeared in a special issue of *BIT*. The papers from the Portugal workshop have just appeared in a special issue of *Optimization in Engineering* edited by Audet, Dennis, and Professor Luis Vicente of Coimbra, who received his PhD with Dennis at Rice.

The statement of work for this add-on contract was mostly concerned with work on combining our new MADS algorithm with the filter method for handling constraints. This has turned out to be a difficult problem, but we are in the process of preparing a paper now on the subject.

We have recently made an important breakthrough in both the theory and the practice of derivative-free methods. Our new research eliminates the main limitation of the Generalized Pattern Search (GPS) class of algorithms, which formed the algorithmic infrastructure for our past work. Our new work addressed the issue that the GPS algorithm class relies heavily on a fixed finite set of directions, and that the convergence results are heavily tied to these directions. We found a way to lift this restriction, and now we allow the algorithm to explore in a set of directions which is dense in the entire space. We call this the Mesh Adaptive Direct Search (MADS) class of algorithm, and it generalizes GPS. We observed significant improvements on some interesting problems.

Lt Col. Abramson, Audet, and Dennis are working to draft a graduate level engineering and applied mathematics textbook based on our research. In addition, Lt Col Abramson is showing himself to be a valuable and active independent researcher. He is our best transition to the USAF. His dissertation is available from www.caam.rice.edu as TR02-11, and several subsequent papers can be found there as well. His NOMADm Matlab implementation of the class of algorithms we study was acknowledged to be the model for the new Matlab toolbox on direct search and genetic algorithms. http://www.mathworks.com/products/gads/description4.jsp

Two students completed the courses, and passed their written B-exams for the Ph.D. in Montréal under the supervision of Audet. Both students work on extensions of MADS: Sébastien Le Digabel's will use parallelism and reduction techniques to allow GPS to tackle larger problems, and Walid Zghal's work will focus on multiobjective and bilevel black box optimization. Audet also supervises a M.Sc. student that specializes MADS to a process optimization problem from chemical engineering.

John Dennis served on the PhD committee of Parvez Moin's Stanford graduate student Alison Marsden, whose dissertation deals with applying the surrogate management framework to obtain quiet trailing edge airfoil designs. We have published two joint papers on this work, and Ms Marsden is presently applying MADS to fully turbulent flow governed by a large eddy simulation. The optimization has been running for six months, and it has achieved an 80% decrease in acoustic noise so far. Dr. Marsden is presently a postdoc in the Stanford Medical School, where her task is to apply our ideas to bioengineering design. We continue to work together.

Accomplishments/New Findings:

Especially noteworthy accomplishments are:

- Several papers have appeared or been accepted by top peer reviewed

journals. Our papers combine theoretical results, analysis of the limitations of GPS and numerical results on some real engineering problems.

- The new MADS framework will replace our GPS framework. MADS is much more flexible, and allows us to show the convergence results that we always wished for in GPS, but knew did not hold. This opens the door for updating all our previous papers into this new framework. This will be done in the book.

- Dennis has taken the lead in developing with Boeing researchers a more mathematical approach to the area called systems of systems. This area has many military and civilian applications. Most of the papers in the literature are written from a systems engineering approach, which Boeing feels is not sufficient to establish a unified approach to algorithms for such problems. Copies of these preprints will be forwarded separately to Dr. Glassman.

Personnel Supported:

Faculty: Professor John Dennis

Publications:

Published:

- Mark A. Abramson, Charles Audet, and J. E. Dennis, Jr. Generalized pattern searches with derivative information. *Mathematical Programming*, Series B, 100:3–25, 2004.

- Charles Audet and J. E. Dennis, Jr. Analysis of generalized pattern searches. *SIAM Journal on Optimization*, 13(3):889–903, 2003.

- Charles Audet and J. E. Dennis, Jr. A pattern search filter method for nonlinear programming without derivatives. *SIAM Journal on Optimization*, 14(4):980–1010, 2004.

- J. E. Dennis, Jr., C. Price and I. Coope) Direct Search Methods for Nonlinearly Constrained Optimization Using Filters and Frames, *Optimization and Engineering* 5(2), pp 123-144, 2004.

- Alison Marsden, Meng Wang, J. E. Dennis, Jr., and Parviz Moin, Optimal aeroacoustic shape design using the surrogate management framework, *Optimization and Engineering*, 5(2):101–122, 2004.

- Alison L. Marsden, Meng Wang, J. E. Dennis, Jr., and Parviz Moin), Suppression of vortex-shedding noise via derivative-free shape optimization (Physics of Fluids), 16(10) 2004, p. L83-L86 2004.

Accepted for Publication:

None at present

Submitted for Publication:

- Mark A. Abramson, Charles Audet, and J. E. Dennis, Jr. Filter pattern search algorithms for mixed variable constrained optimization problems. Technical Report TR04-09, CAAM technical report, Rice University, 2004. submitted to Pacific Journal of Optimization.

- Mark A. Abramson, Olga A. Brezhneva, and J. E. Dennis, Jr. Pattern Search Methods for Linearly Constrained Minimization in the Presence of Degeneracy, IMA Preprint series, # 1934, and Rice CAAM-TR03-09, August 2003.

- Charles Audet and J. E. Dennis, Jr. Mesh adaptive direct search algorithms for constrained optimization. Technical Report G–2004–04, Les Cahiers du GERAD, 2004. submitted to SIAM JOPT.

Interactions and Transitions:

Public Presentations:

J. E. Dennis

- "Optimization using Surrogates for Engineering Design". Departmental Colloquium, Mechanical Engineering Department, University of Michigan, Ann Arbor, April 16, 2004.
- "Optimization using Surrogates for Engineering Design". RODD AFOSR Meeting, Shalimar Florida, April 20, 2004.
- "Mesh Adaptive Direct Search Algorithms". AFOSR Program Review, Pasadina, California, August 11, 2004.
- "Mesh Adaptive Direct Search Algorithms". Optimization seminar, University of Wisconsin, Madison, September 23, 2004.
- "Optimization using Surrogates for Engineering Design". Departmental Colloquium, Industrial Engineering Department, University of Wisconsin, Madison, September 24, 2004.
- "Optimization Using Surrogates for Engineering Design." Boeing Distinguished Scholar Series, Webcast company wide, December 2, 2004.
- "Optimization using Surrogates for Engineering Design". Industrial Mathematics Series, Fields Institute for Mathematics, University of Toronto, February 1, 2004
- "Mesh Adaptive Direct Search Algorithms". Optimization seminar, MacMaster University, Hamilton, Ontario, February 3, 2004.
- "Mesh Adaptive Direct Search Algorithms". Optimization seminar, ExxonMobil Upstream Research, Houston, February 10, 2005.
- "Mathematical Formulations of Systems of Systems Problems". ExxonMobil Upstream Research, Houston, February 11, 2005.

- "Optimization using Surrogates for Engineering Design". West Coast Optimization Meeting, University of Washington, Seattle, April 30, 2005.

Editorial positions:

J. E. Dennis

2001–	Editorial Board, *SIAM Journal on Optimization*
1992–	Advisory Editor, *Mathematics of Operations Research*
2003–2004	Invited Editor for *Optimization and Engineering* (special issue on Surrogate Optimization)

Consultative and Advisory Functions:

J. E. Dennis

- Renewal site visit team for NSF Institute for Pure and Applied Mathematics at UCLA, October 2004.
- One day per week at Boeing Phantom Works Mathematics and Engineering Analysis Group working on Design Explorer Project and Systems of Systems optimization.
- Advisory Committee for Worcester Polytechnic Institute.
- ExxonMobil Upstream Research Company
- United Technologies Research Center
- Lawrence Berkeley Laboratory Nanotechnology project.

- Served on PhD committee for Stanford University Mechanical Engineering doctoral candidate Alison Marsden.

Transitions:

Projects in the Exploratory Stage

- Systems of Systems With a group of Boeing collaborators, we are looking at systems of systems problems from a mathematical point of view. Previous work has come mostly from the military operations research community, and it has been largely concerned with ad hoc solutions of specific cases. We have written a Boeing Technical Report (nonproprietary), which has been invited for presentation at the upcoming IEEE meeting on Systems of Systems. We are almost finished with another more general paper. Our approach is to categorize SoS problems depending on the degree of control exercised by the "central authority" ranging from inactive to omnipotent.

  Contact: Dr. Evin Cramer (206)232-9577 or
  Dr. Greg Shubin (425)865-3516.

- **Well casing** All of the personnel who received support from this grant spent some time at ExxonMobil Upstream Research Company talking about various collaborations. One problem presently being discussed is an interesting mixed integer problem, which is described briefly as follows. As a well is being drilled, it is important to insert sleeves of well casing to keep the sides of the hole from collapsing into the well. The first sleeve is the largest in diameter, the second is inserted inside the first and lowered into place, and this concentric sleeving continues until the drilling is completed and the wall of the well is completely reinforced by concentric sleeves of decreasing diameter. The problem is to determine the number of sleeves, a categorical variable, and the length and diameter of each sleeve for a well of given depth. Of course, there are various structural constraints, and cost is the objective to be minimized. We should be able to deal with this problem with little

difficulty, but the delay is due to a need to obtain internal funding for ExxonMobil personnel to gather all the necessary simulation routines. The status of this project is that NOMAD has been successfully used by ExxonMobil to solve the problem for a single section.

Contact: Dr. Amr ElBakry (713)431-7137.

- **Nozzle Design** Our group continues working with a group in Boeing Commercial Airplane Group (BCAG) to reduce the cycle time for designing nozzles. A nozzle is the inside part of the engine housing, and its design is affected by the design of the more "upstream" components. This means that many of the design changes involving other airplane components force a redesign of the nozzle as well.

  A nozzle design is specified by 100 parameters, 90 of which are fixed by other considerations. The system is governed by a 2D Navier Stokes coupled with NASTRAN, a commercial structures code. It takes about 3 hours on an SGI Challenge to get one function value. The current length of a design cycle is two weeks. We expect to reduce that to approximately one day.

  This project has been delayed by the higher internal Boeing priority of the planform project.

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Ongoing Projects

- **Model Management Framework Software** Boeing has the latest NOMAD-C++ release as well as the NOMADm MatLab software. When internal funding permits, this will likely become the basis for reimplementation of their Design Explorer Software. This implementation replaces the C++ box constrained prototype delivered previously. The framework can be used to develop model management algorithms specialized for a user's applications and capabilities. The Boeing version of our work, Design Explorer, is presently being commercialized by Phoenix Integration.

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- **Planform Design** Our algorithms were used in a production environment by Boeing in planform design for the near sonic cruiser. This was done by the BCAG group that does planform design. The decision was made not to build this airplane because of economic conditions in the airline industry. Now, Design Explorer is being used on the proposed Dreamliner 7e7. Boeing continues to achieve better planforms with greatly reduced cycle time.

  The planform is the shape of the wing as viewed from above. It is a tricky design problem that involves a couple of dozen variables and some interesting constraints. For example, the fuel is outboard on the wings, and the wings must be swept back for performance. One constraint is that the plane must not fall over backwards when the tanks are filled while the plane is on the ground. This problem involves multiple objectives and discrete variables, but the first test problem run by Boeing used cost/passenger mile as objective and assumed values for the discrete variables, like where the wings are placed on the body.

  The following text on the recent test was approved by Boeing for release:

  Recent Product Development activities at Boeing have underscored the need to decrease the time to market and cost of products. To accomplish this, Boeing has been examining all of its processes in development and production.

  One process in particular that occurs early in the design is the determination of a wing planform, which must be chosen to meet mission while decreasing operating economics and respecting design constraints. Boeing is exploring whether this highly multi-disciplinary problem yields itself to integrated analysis and optimization techniques, with the hope of decreasing the cycle time of finding a preferred result by an order of magnitude.

  This exploration provided the Design Explorer Team, of which Rice is a member, with an opportunity to apply our design optimization tools. It has also been useful from the standpoint of exercising the various discipline analysis tools. Starting from baselines developed through the standard process and using a significant subset of the tools, we

have been able to demonstrate actual integration of the analyses from the different disciplines and the speed advantages that we were looking for. The solutions found do, within the level of accuracy of the included tools, meet all constraints while showing economic benefit relative to our analyses of the initial baselines.

The approach to this problem used response surface (surrogate) modeling to speed up the optimization, as opposed to continuously resampling the analysis tools. Of additional note is that incorporation of Model Management Framework elements into the optimization scheme allowed resolution of the selected optimum to search variables of second order importance. Such resolution is particularly difficult to obtain when using response surface modeling.

Contact: Dr. Evin Cramer (206)232-9577 or
Dr. Greg Shubin (425)865-3516.

- **Boeing Parts Nesting System** PDS continues to be used in the Boeing Parts Nesting System 2NA for just-in-time manufacturing of aircraft parts. This code runs over 100,000 times per day.

- **Optimal algorithmic parameters** We devised a general framework for parameter tuning that uses MADS to identify good algorithmic parameters. The framework makes provision for surrogate objectives. Parameters are sought so as to minimize some measure of performance of the algorithm being fine-tuned. This measure is treated as a black-box and may be chosen by the user.

  We specialized this framework to the identification of trust-region parameters in unconstrained optimization. Parameters are identified that minimize, in a certain sense, the computational time or the number of function evaluations required to solve a set of problems from the CUTER collection. Each function call may take several hours and may not always return a predictable result. A surrogate function, tailored to the experiment at hand, is used to guide MADS towards a local solution.

  Contact: Dr. Dominique Orban (514)340-4711 ext 5967

- **Trailing edge design** We have a collaboration with Parviz Moin's turbulent flow group in the Mechanical Engineering Department at Stanford. Our algorithms have been successful in achieving airfoil designs

with over 50% reduction in noise from flow over the wings. There are several important application of this work from windmills to aircraft.

Contact: Dr. Alison Marsden (650) 723-2416

Inventions, or Patent Disclosures:

None.

Honors/Awards:

J. E. Dennis

- Very Important Visitor at Institute for Mathematics and its Applications at the University of Minnesota Winter 2003
- Ordway Distinguished Lecturer in the Mathematics Department at the University of Minnesota Winter 2003
- Chair of the organizing committee for the SIAM 2004 Annual Meeting, August, Portland, OR
- Named a HighlyCited Computer Scientist by ISI.
- Dedicatee of special issue of the *SIAM Journal on Optimization* (Volume 9, Number 4) <http://epubs.siam.org/sam-bin/dbq/toc/SIOPT/9/4>.
- Chair(President) of the Mathematical Programming Society
- Founder and Editor-in-Chief of MPS/SIAM Book Series on Optimization
- Advisory Editor, *Mathematics of Operations Research*, (1992—).

- Founding Editor-In-Chief of *SIAM Journal on Optimization.*
- Served on and chaired numerous panels and visiting committees.
- Served two terms on the SIAM Council.
- Fulbright Lecturer to Argentina.
- Three times an Erskine Fellow at the University of Canterbury, Christchurch, NZ, 2000, 2002, and 2004.